4.0 FLAME-RETARDANT ALTERNATIVES EVALUATIONS

In order to evaluate chemical alternatives for flame retarding furniture foam, all of the factors discussed in prior sections of this report must be considered, including toxicology, exposure, type of flame-retardant chemical, efficacy of use within existing manufacturing systems, availability and viability of non-chemical alternatives, cost and performance. This report does not include information on performance testing or cost.

This section summarizes the toxicological and exposure characteristics of each chemical in alternative flame-retardant formulations that are considered viable substitutes for pentaBDE use in flexible polyurethane foam. Chemical components less than 1 percent by weight were not considered in this assessment. The characteristics of the chemicals in each formulation are summarized qualitatively in Section 4.1 using a relative ranking scheme and more detailed characteristics of the chemicals in each formulation are presented in Section 4.2.

These evaluations of flame-retardants are not full risk assessments, but do provide screening-level information on the hazard concerns and potential routes of exposure associated with the chemical components. Chemical risk is composed of two parts: hazard and exposure. The hazards evaluated in this report were the potential for human health effects and ecotoxicity. Exposure refers to the amount of material to which workers, the community or the environment come into contact. The toxicological information summarized in these evaluations is based on existing information and will provide the basis for identifying unmet data needs. The exposure potential is derived from simple criteria applied to the physical, chemical, and environmental fate properties of the chemicals. A full exposure assessment would consider the quantity, frequency, duration and route of exposure. Understanding the exposure routes and pathways is critical to conducting an exposure assessment. The concentration of a chemical in the mixture would factor into the overall exposure assessment and, therefore, the potential risk associated with the commercial formulations of the flame retardant alternatives.

4.1 Summary of Flame-Retardant Chemical Alternatives

Table 4-1 presents a qualitative summary of toxicological and exposure characteristics of the chemicals in each formulation considered in the alternatives analysis. The table qualitatively summarizes toxicological endpoints and exposure routes for each chemical, including seven human health effects, two ecotoxicity effects and two environmental endpoints and six routes of occupational, general population and aquatic exposure. Each of these endpoints is explained in Table 4-2.

Each toxicological endpoint in Table 4-1 is assigned a rating of L, M, or H to indicate whether the chemical has a low (L), medium (M), or high (H) hazard concern. If the L, M, or H indicator is bold or colored, then the assignment was made using experimental data on the chemical. If the L, M, or H indicator is italicized, then experimental data were not available for that chemical and the assignment was estimated using structure activity relationships (SAR) analysis involving modeling techniques and professional judgment. Similarly, each exposure route is assigned a rating of Y (yes) or N (no) to indicate whether that exposure route may occur for each chemical.

Table 4-1 Screening Level Toxicology and Exposure Summary

L = Low hazard concern
M[1] = Moderate hazard concern
H = High hazard concern
N = No
Y = Yes
P = Yes for pure chemical
*Ongoing studies may result in a change in this endpoint
▲Persistent degradation products expected[2]
L, M[1], or *H* = Endpoint assigned using estimated values and professional judgment (Structure Activity Relationships)

Company	Chemical`	% in Formulation[3]	Human Health Effects							Ecotoxicity		Environmental		Potential Routes of Exposure							Reactive or Additive?
														Worker			General Population				
			Cancer Hazard	Skin Sensitizer	Reproductive	Developmental	Neurological	Systemic	Genotoxicity	Acute	Chronic	Persistence	Bioaccumulation	Inhalation	Dermal	Ingestion	Inhalation	Dermal	Ingestion	Aquatic	
Albemarle	ANTIBLAZE 180 and ANTIBLAZE 195																				
	Tris(1,3-dichloro-2-propyl)Phosphate CAS # 13674-87-8	95%	M	L	M	M	L	M	M	M	M	M	*L*	N	Y	Y	N	Y	Y	Y	Additive
Albemarle	ANTIBLAZE 182 and ANTIBLAZE 205																				
	Proprietary A Chloroalkyl phosphate (1)		M	L	M	M	L	M	M	M	M	M	*L*	N	Y	Y	N	Y	Y	Y	Additive
	Proprietary B Aryl phosphate		*L*	*L*	M*	M*	M	M*	*L*	H	*H*	*L*	*M*	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		*L*	L	L	L	L	M	L	H	*H*	L	L	Y	Y	Y	Y	Y	Y	Y	Additive
Albemarle	ANTIBLAZE V500																				
	Proprietary C Chloroalkyl phosphate (2)		*M*	M	*M**	*M**	L	M	L	M	M	M	*L*	N	Y	Y	N	Y	Y	Y	Additive
	Proprietary B Aryl phosphate		*L*	*L*	M*	M*	M	M*	*L*	H	*H*	*L*	*M*	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		*L*	L	L	L	L	M	L	H	*H*	L	L	Y	Y	Y	Y	Y	Y	Y	Additive
Albemarle	SAYTEX RX-8500																				
	Proprietary D Reactive brominated flame retardant		*L*	*M*	*L*	*L*	*M*	*M*	L	*M*	*M*	*L*▲	*L*	N	Y	Y	N	N	Y	Y	Reactive
	Proprietary B Aryl phosphate		*L*	*L*	M*	M*	M	M*	*L*	H	*H*	*L*	*M*	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		*L*	L	L	L	L	M	L	H	*H*	L	L	Y	Y	Y	Y	Y	Y	Y	Additive

[1] The moderate designation captures a broad range of concerns for hazard.
[2] More information on degradation products can be found in sections 4.1.1 and 5.1.
[3] Chemical concentrations are listed in descending order; only chemicals with concentrations greater than one percent in the formulation were evaluated.

Table 4-1 Screening Level Toxicology and Exposure Summary

L = Low hazard concern
M[4] = Moderate hazard concern
H = High hazard concern
N = No
Y = Yes
P = Yes for pure chemical
*Ongoing studies may result in a change in this endpoint
▲Persistent degradation products expected[5]
L, M[1], or *H* = Endpoint assigned using estimated values and professional judgment (Structure Activity Relationships)

Company	Chemical	% in Formulation[6]	Human Health Effects							Ecotoxicity		Environmental		Potential Routes of Exposure							Reactive or Additive?
														Worker			General Population				
			Cancer Hazard	Skin Sensitizer	Reproductive	Developmental	Neurological	Systemic	Genotoxicity	Acute	Chronic	Persistence	Bioaccumulation	Inhalation	Dermal	Ingestion	Inhalation	Dermal	Ingestion	Aquatic	
Albemarle	SAYTEX RZ-243																				
	Proprietary E Tetrabromophthalate diol diester		*L*	*L*	*L**	*L**	*L*	*M**	*L*	*L*	*H*	*L*▲	*L*	N	Y	Y	N	N	Y	Y	Additive
	Proprietary B Aryl phosphate		*L*	*L*	M*	M*	M	M*	*L*	H	*H*	*L*	*M*	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		*L*	L	L	L	L	M	L	H	*H*	L	L	Y	Y	Y	Y	Y	Y	Y	Additive
Ameribrom	FR513																				
	Tribromoneopentyl Alcohol CAS # 36483-57-5		*M*	L	*M*	*M*	*M*	M	M	M	*M*	L	*L*	Y	Y	Y	N	N	Y	Y	Reactive
Great Lakes	Firemaster 550																				
	Proprietary F Halogenated aryl ester		*L*	*L*	*M*	*M*	*L*	*M*	*L*	H	*H*	L▲	L	N	Y	Y	N	Y	Y	Y	Additive
	Proprietary G Triaryl phosphate, isopropylated		*L*	*L*	M*	M*	M	M*	*L*	H	*H*	*L*	*M*	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		*L*	L	L	L	L	M	L	H	*H*	L	L	Y	Y	Y	Y	Y	Y	Y	Additive
	Proprietary H Halogenated aryl ester		*L*	*L*	*M*	*M*	*L*	*M*	*L*	H	*H*	L▲	L	N	Y	Y	N	Y	Y	Y	Additive
Great Lakes	Firemaster 552																				
	Proprietary F Halogenated aryl ester		*L*	*L*	*M*	*M*	*L*	*M*	*L*	H	*H*	L▲	L	N	Y	Y	N	Y	Y	Y	Additive
	Proprietary G Triaryl phosphate, isopropylated		*L*	*L*	M*	M*	M	M*	*L*	H	*H*	*L*	*M*	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		*L*	L	L	L	L	M	L	H	*H*	L	L	Y	Y	Y	Y	Y	Y	Y	Additive
	Proprietary H Halogenated aryl ester		*L*	*L*	*M*	*M*	*L*	*M*	*L*	H	*H*	L▲	L	N	Y	Y	N	Y	Y	Y	Additive

[4] The moderate designation captures a broad range of concerns for hazard.
[5] More information on degradation products can be found in sections 4.1.1 and 5.1.
[6] Chemical concentrations are listed in descending order; only chemicals with concentrations greater than one percent in the formulation were evaluated.

Table 4-1 Screening Level Toxicology and Exposure Summary

L = Low hazard concern
M[1] = Moderate hazard concern
H = High hazard concern
L, M*[1]*, or H = Endpoint assigned using estimated values and professional judgment (Structure Activity Relationships)

N = No
Y = Yes
P = Yes for pure chemical

*Ongoing studies may result in a change in this endpoint
▲Persistent degradation products expected[2]

Company	Chemical	% in Formulation[3]	Human Health Effects							Ecotoxicity		Environmental		Potential Routes of Exposure							Reactive or Additive?
														Worker			General Population				
			Cancer Hazard	Skin Sensitizer	Reproductive	Developmental	Neurological	Systemic	Genotoxicity	Acute	Chronic	Persistence	Bioaccumulation	Inhalation	Dermal	Ingestion	Inhalation	Dermal	Ingestion	Aquatic	
Supresta	AB053																				
	Tris(1,3-dichloro-2-propyl)Phosphate CAS # 13674-87-8		M	L	M	M	L	M	M	M	M	M	*L*	N	Y	Y	N	Y	Y	Y	Additive
Supresta	AC003																				
	Proprietary I Organic phosphate ester	92-99%	*L*	L	L	L	*L*	*M*	L	H	H	H	L	P	Y	Y	N	Y	Y	Y	Additive
	Triphenyl Phosphate CAS # 115-86-6	1-8%	*L*	L	L	L	L	M	L	H	*H*	L	L	Y	Y	Y	Y	Y	Y	Y	Additive
Supresta	AC073																				
	Triphenyl Phosphate CAS # 115-86-6	38-48%	*L*	L	L	L	L	M	L	H	*H*	L	L	Y	Y	Y	Y	Y	Y	Y	Additive
	Proprietary J Aryl phosphate	40-46%	*L*	*L*	L	*L*	L	M	M*	*L*	*H*	L	*L*	Y	Y	Y	Y	Y	Y	Y	Additive
	Proprietary K Aryl phosphate	12-18%	*L*	*L*	*L*	*L*	*L*	*M*	*L*	*L*	*L*	*L*	*L*	P	Y	Y	N	Y	N	N	Additive
	Proprietary L Aryl phosphate	1-3%	*L*	*L*	*L*	*L*	*L*	*M*	*L*	*L*	*L*	*L*	*L*	P	Y	Y	N	Y	N	N	Additive
Supresta	Fyrol FR-2																				
	Tris(1,3-dichloro-2-propyl)phosphate CAS # 13674-87-8	99%	M	L	M	M	L	M	M	M	M	M	*L*	N	Y	Y	N	Y	Y	Y	Additive

[1] The moderate designation captures a broad range of concerns for hazard.
[2] More information on degradation products can be found in sections 4.1.1 and 5.1.
[3] Chemical concentrations are listed in descending order; only chemicals with concentrations greater than one percent in the formulation were evaluated.

Table 4-2 Definitions of Toxicological and Environmental Endpoints

Toxicological Category	Toxicological Endpoint	Definition
Human Health Effects	Cancer Hazard	Any growth or tumor caused by abnormal and uncontrolled cell division.
	Skin Sensitizer	Chemical that causes an allergic skin reaction characterized by the presence of inflammation; may result in cell death.
	Reproductive	Adverse effects on the reproductive systems of females or males, including structural/functional alterations to the reproductive organs/system, the related endocrine system, mating, or fertility/reproductive success.
	Developmental*	Adverse effects on the developing organism (including structural abnormality, altered growth, or functional deficiency or death) resulting from exposure prior to conception (in either parent), during prenatal development, or postnatally up to the time of sexual maturation.
	Neurological	Adverse effects on the central or peripheral nervous system.
	Systemic	Adverse effect (other than those listed separately) that is of either a generalized nature or that occurs at a site distant from the point of entry of a substance: a systemic effect requires absorption and distribution of the substance in the body.
	Genotoxicity	Induction of genetic changes in a cell as a consequence of gene sequence changes (mutagenicity), or chromosome number/structure alterations.
Ecotoxicity	Adverse effects observed in living organisms that typically inhabit the wild. The assessment focused on effects in aquatic organisms (fish, invertebrates, algae).	
	Acute	Short-term, in relation to exposure or effect. Exposures are typically less than 96 hours.
	Chronic	Effects observed after repeated exposures.
Environmental	Persistence	Attribute of a substance that describes the length of time that the substance remains in the environment before it is physically removed by chemical or biological transformations.
	Bioaccumulation*	Ability of living organisms to concentrate a substance obtained either directly from the environment or indirectly through its food.

*REFERENCE: International Union of Pure and Applied Chemistry, Clinical Chemistry Division Commission on Toxicology. Glossary for Chemists of Terms Used in Toxicology (IUPAC Recommendations, 1993).

4.1.1 Explanation of Toxicological and Environmental Endpoints Rating

The assessments combine data on flame-retardant alternatives from four sources: (1) publicly available measured (experimental) data obtained from a comprehensive literature review; (2) measured confidential data from EPA OPPT Confidential Business Information (CBI) databases; (3) SAR-based estimations from EPA's New Chemical Program's P2 Framework and Sustainable Futures predictive methods; (4) professional judgment of EPA staff who identified experimental data on closely related analogs; and (5) confidential studies submitted by chemical manufacturers. When experimental data were lacking, the expert judgment of scientists from EPA's New Chemical Program was used to assess physical/chemical property, environmental fate, aquatic toxicity and human health endpoints. The following abbreviations are used to indicate sources of data presented in this assessment:

- M = Measured/experimental data contained in the open literature;
- MC = Measured/experimental confidential data contained in EPA OPPT CBI databases or submitted by industry;

- E = Estimations obtained using predictive methodology; and
- P = Professional judgment of subject matter experts.

Table 4-3 lists the criteria that were used to interpret the data collected in this document. These criteria are used by the EPA New Chemicals Program to assign concern levels to new chemicals submitted under the Toxic Substances Control Act (TSCA). EPA has published these criteria in several sources including USEPA 1992, USEPA 1994, and USEPA 1995. EPA New Chemicals Program persistence criteria have been published in the Federal Register (USEPA 1999).

Table 4-3 Criteria Used to Assign Concern Levels

Concern Level	**Persistence Criteria**
High	Half-life in water, soil, or sediment > 180 days
Moderate	Half-life in water, soil, or sediment between 60 and 180 days
Low	Half-life in water, soil, or sediment < 60 days
Concern Level	**Bioaccumulation Criteria**
High	Bioconcentration factor (BCF) > 5000
Moderate	BCF between 1,000 and 5,000
Low	BCF < 1,000
Concern Level *	**Aquatic Toxicity Criteria**
High	Value is ≤ 1 mg/L (chronic value <0.1 mg/L)
Moderate	Value is between 1 and 100 mg/L (chronic value 0.1 and 10 mg/L)
Low	Value is >100 mg/L (chronic value >10 mg/L) or log K_{ow} is greater than 8
Concern Level	**Human Health Criteria**
High	Evidence of adverse effects in human populations *or* conclusive evidence of severe effects in animal studies
Moderate	Suggestive animal studies, analog data, *or* chemical class known to produce toxicity
Low	No basis for concern identified

*If the water solubility is estimated, the chemical will not be considered to have "no effects at saturation" if the estimated value is within a factor of 10 percent of the cutoff value. The concern level will be considered low if "no effects at saturation" (below the solubility limit).

More information on the EPA New Chemicals Program criteria used to assign concern levels can be found in the Sustainable Futures Pilot Project Interpretive Guidance Document (attached as Appendix B to this document) or visit: http://www.epa.gov/oppt/newchems/sustainablefutures.htm.

There are many other hazard classification systems which can be applied to the experimental data listed in Section 4.2 and Volume II of this report. Examples of these systems include.

- Globally Harmonized System of Classification and Labelling of Chemicals (GHS)
  http://www.unece.org/trans/danger/publi/ghs/ghs_rev00/00files_e.html

- EPA's Office of Pesticide Programs (OPP)
  A comparison of the OPP criteria and GHS criteria:
  http://www.epa.gov/oppfead1/international/global/ghscriteria-summary.pdf

- EU Dangerous Substance Directive (EU)
  Links to the directive, annexes and all amendments can be found here:
  http://europa.eu.int/comm/environment/dansub/main67_548/index_en.htm

- Annex 6 lists the general labeling and classification requirements for dangerous substances and preparations:
  http://europa.eu.int/comm/environment/dansub/pdfs/annex6_en.pdf

- Canadian Hazardous Products Act (Canada)
  The Consumer Chemical Container Regulations:
  http://laws.justice.gc.ca/en/H-3/SOR-2001-269/text.html

- The Controlled Products Regulations:
  http://laws.justice.gc.ca/en/H-3/SOR-88-66/text.html

If measured data pertaining to these criteria are not available, they can be estimated based on use of Structure Activity Relationships (SAR) analysis. SAR is the relationship of the molecular structure of a chemical with a physicochemical property, environmental fate attribute, and/or specific effect on human health or an environmental species. These correlations may be qualitative (simple SAR) or quantitative (quantitative SAR, or QSAR). Information on EPA's use of SAR analysis has been published in USEPA 1994.

SAR estimations for several physical and chemical properties were obtained using the models of EPA's P2 Framework. The P2 Framework is an approach to risk-screening that incorporates pollution prevention principles in the design and development of chemicals. These models are screening level methods and are intended to be used when data are unavailable or to supplement available data. They are not intended to replace data from well-designed studies. For physical/chemical properties and environmental fate parameters, estimates were obtained from the Estimations Program Interface for Windows (EPIWIN) suite methodology. These methods were used to obtain melting point, boiling point, vapor pressure, octanol/water partition coefficient, water solubility, Henry's Law constant, atmospheric oxidation rate, biodegradation potential, soil adsorption coefficient, bioconcentration factor, hydrolysis rate, volatilization rates and removal in a sewage treatment plant as applicable. For aquatic toxicity potential, EPA's Ecological Structure Activity Relationships (ECOSAR) estimation program was used. This methodology uses chemical structure to estimate toxicity of an industrial chemical to fish, invertebrates, and algae in the surface water to which the chemical has been discharged. The program determines both acute (short-term) toxicity and, when available, chronic (long-term or delayed) toxicity. The potential for a chemical to cause cancer in humans was estimated using OncoLogic. This program uses a decision tree based on the known carcinogenicity of chemicals

with similar chemical structures, information on mechanisms of action, short-term predictive tests, epidemiological studies, and expert judgment. All estimates obtained in this project were reviewed by EPA scientists with expertise in the appropriate field.

The persistence of a chemical substance in a screening assessment is based on determining the importance of removal processes that may occur once a chemical enters the environment. As noted above, chemicals with a half-life of less than 60 days are expected to be of low concern for persistence based on the criteria that were used to interpret the data collected in this document. The persistence screening assessment does not directly address the pathways that a flame retardant might enter the environment (e.g., volatilization or disposal in a land fill) and focuses instead on the removal processes that are expected to occur once it is released to air, water, soil, or sediment. Determining how a chemical enters the environment is typically a component of a complete exposure assessment or life cycle analysis and is discussed in Section 3. Similarly, the persistence screening assessment does not address what might happen to a chemical substance throughout its life cycle, such as disposal during incineration of consumer or commercial products (incineration is discussed briefly in Section 5.1).

Environmental removal processes are generally divided into two categories: chemical and biological. One of the most important chemical degradation processes is hydrolysis. The importance of hydrolysis can be determined from experimental data (on both the compound of interest and closely related analogs) and by using the half-life obtained from the models within EPIWIN. Photolysis may also be an important environmental removal process and was considered in this assessment when experimental data were available. Estimation methods for photolysis are not available within EPA's Sustainable Future pilot project.

Biodegradation is also considered in determining the persistence of a chemical substance in the environment. If experimental data on the biodegradation of a chemical substance are not available, then the potential of the chemical to undergo this process can be assessed from the results of the EPIWIN models. These models fall into three classes:

1. Probability of rapid biodegradation models based on linear and non-linear regressions that estimate the probability that a chemical substance will degrade fast;

2. Expert survey models – semi-quantitative models that determine the rate of ultimate and primary biodegradation; and

3. Probability of ready biodegradability.

The first set of models are useful for determining if a chemical substance has the potential to biodegrade quickly in the environment, but do not provide a quantitative indication of its half-life. If a chemical is likely to biodegrade quickly its half-life is expected to be less than 60 days and, therefore, it is expected to have a low concern for persistence. The results of the estimates from the first set of models are used in concert with the semi-quantitative output from the second set of models, which include an ultimate and primary survey model for evaluating persistence. These models provide a numeric result, ranging from 1 to 5, to provide an indication of the amount of time required for complete mineralization (ultimate degradation) and removal of the parent substance (primary degradation) of the test compound. The numeric result is converted to

a more meaningful time frame for removal for the user based on the scheme presented in the following table. The results from the ultimate degradation model can also be used to estimate the half-life for a chemical, which is also provided in Table 4-4.

Table 4-4 Information for Estimating Half-Life

Model Results for Primary and Ultimate	Time for Removal	Approximate Half-Life (Days, Based on ultimate)
>4.75	Hours	0.17
4.75 to >4.25	Hours to Days	1.25
4.25 to >3.75	Days	2.33
3.75 to >3.25	Days to Weeks	8.67
3.25 to >2.75	Weeks	15
2.75 to >2.25	Weeks to Months	37.5
2.25 to >1.75	Months	60
≤1.75	Recalcitrant	180

The third set of models (also known as MITI models), and the ready biodegradability test that they correspond to, are more applicable to determining a chemical's potential for removal in a sewage treatment plant than its persistence in the environment.

When determining environmental persistence, screening assessments also consider the potential persistence of breakdown products resulting from biodegradation and chemical removal processes. This assessment is performed because of the potential for human and environmental exposure to persistent breakdown products. Breakdown products resulting from hydrolysis can be determined experimentally or by using professional judgment based on analogs with similar functional groups. Breakdown products may also be reported in experimental biodegradation tests or can be determined using professional judgment. When the rate for ultimate degradation is much slower than that for primary degradation, the potential for persistent breakdown products exists.

4.1.2 Explanation of Exposure Route Rating

Six exposure routes are presented for each chemical, including two occupational exposure routes, three general population exposure routes and one aquatic exposure route. Each of these potential routes is assigned a Y (yes, exposure may occur) or an N (no, exposure is not likely to occur). The potential for occupational exposure is determined by the physicochemical properties of the pure material. If the flame retardant is commonly manufactured or formulated as a liquid and the vapor pressure indicates that it is not expected to volatilize, then a "P" indicates that the potential for worker inhalation exposure is expected to be limited to those situations when the material is in a purified form that could contribute to dust-related exposure. The exposure routes are based on the state of the pure compound or representative pure compound unless further use information has been provided. The thresholds for each exposure route were adapted from EPA's New Chemicals Program, except as noted.

Occupational Exposure

Inhalation

Liquids[4]: If a liquid has a vapor pressure amenable to volatilization, then the liquid will evaporate and present the potential for a person to inhale the vapor. Occupational exposure may occur when the vapor pressure is greater than 1×10^{-06} mm Hg at 25 degrees Celsius. Liquids may also be inhaled as a mist if the liquid chemical is sprayed during transfer or application operations.

Solids[5]: Occupational exposure may occur in all cases when processing or handling solids. Solid-state chemicals may be used in a crystalline, packed, or powder form. In all cases, a solid chemical may produce particulate dust as a byproduct of manufacturing or use operations. When this occurs, a worker may inhale the dust particles while working with the chemical.

Gases[6]: Occupational exposure may occur in all cases when processing or handling gases. Gaseous chemicals should always be contained in cylinders to enable their use; however, if they are uncontained, gaseous chemicals result in exposure to workers. Routine exposure to gaseous chemicals is not expected unless there is an accident. However, fugitive releases may occur when connecting transfer lines.

Dermal

Dermal exposures may occur to workers while handling liquid or solid flame-retardant chemicals. In general, workers handling liquid chemicals may be exposed to the chemical by full hand immersion, splashing, or spraying depending upon the manufacturing processes utilized at a facility. Workers handling solid chemicals can be exposed on the surface of their hands as well as from particulate dust that may settle onto their skin. All chemicals are expected to present a dermal exposure to workers in this report. The use of personal protective equipment may mitigate these exposures.

Ingestion

Exposures associated with ingestion are not included for the purposes of this screening level assessment; however, workers may incidentally ingest flame-retardant chemicals through ingestion of contaminated food and water. Ingestion may occur if the chemical is suspended in air as a particulate or a mist as part of manufacturing, and then recondenses or flocculates into food or drinking sources. Alternatively, secondary ingestion may occur as a result of inhaling the mist or dust form of the chemical, and then swallowing residual chemical in the nasal or esophageal passageways.

[4] Liquids are substances that have a melting point less than 25 degrees Celsius and a boiling point greater than 25 degrees Celsius.
[5] Solids are substances that have a melting point of greater than 25 degrees Celsius.
[6] Gases are substances that have a boiling point less than 25 degrees Celsius.

General Population Exposure

Inhalation

Liquids[7]: If the liquid has a vapor pressure amenable to volatilization from the product in which the chemical is carried, a person may inhale the liquid as a vapor while in contact with the product or substance carrying the chemical. For this report, general population exposure may occur if the chemical vapor pressure is greater than 1×10^{-06} mm Hg at 25 degrees Celsius and if the chemical is additive, not reactive[8].

Solids[9]: General population exposure may occur if the vapor pressure is greater than 1×10^{-06} mm Hg at 25 degrees Celsius and if the chemical is not reactive. Although not included in this screening level assessment, as foam products age and break down, particulate (matter) may be released from the foam products which may contain flame-retardant chemicals. This flame-retardant foam dust may be present in carpets or in flame-retardant furniture and could represent an exposure to the general population.

Gases[10]: General population exposure is not expected to occur if the chemical is a gas, since gases would not be intentionally contained outside of the manufacturing arena (excluding accidental releases).

Dermal

Dermal exposures may occur to the general population while handling products or substances containing the flame-retardant chemical, if the flame-retardant chemical is not reactive.

Ingestion

The general population may be exposed to a flame-retardant chemical if the chemical has water solubility greater than 1×10^{-06} grams/liter, is dispersible, or has the potential to leach. These would indicate that the chemical is easily absorbed in water and may be found in surface and groundwater sources as a result of disposal and environmental releases of the chemical.

Aquatic Exposure

The flame-retardant chemical may present an aquatic exposure if the water solubility of the compound is greater than 1×10^{-06} grams/liter or the compound is dispersible in water.

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[7] Liquids are substances that have a melting point less than 25 degrees Celsius and a boiling point greater than 25 degrees Celsius.

[8] Reactive chemicals (as opposed to additive chemicals) are those that are incorporated into the foam by new chemical bonds that are formed between the substrate and the flame retardant. Therefore, they are not assumed to be available for exposure.

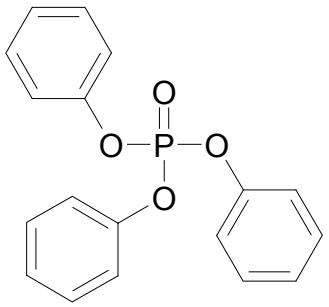
[9] Solids are substances that have a melting point of greater than 25 degrees Celsius.

[10] Gases are substances that have a boiling point less than 25 degrees Celsius.

4.2 Chemical Summary Assessments

The following subsections (4.2.1 through 4.2.19) contain summaries of the toxicity and exposure data for 15 chemicals that are components of the flame retardant formulations assessed in this report. These summary data were used to develop the hazard concern and exposure conclusions that are presented in Table 4-1. The studies from which these data were derived are summarized in Volume 2 of this report, entitled Chemical Hazard Reviews.

4.2.1 Triphenyl Phosphate

<table>
<tr><td colspan="3">Record ID: Triphenyl Phosphate</td><td>CAS No. 115-86-6</td></tr>
<tr><td colspan="3" rowspan="3">  </td><td>MW: 326.29</td></tr>
<tr><td>MF: $C_{18}H_{15}O_4P$</td></tr>
<tr><td>Physical Forms:
Neat: Solid
As Formulated:</td></tr>
<tr><td colspan="3">SMILES: c1ccccc1OP(=O)(Oc2ccccc2)Oc3ccccc3</td><td>Use: Flame retardant, additive</td></tr>
<tr><td colspan="4">Name: Phosphoric acid, triphenyl ester</td></tr>
<tr><td colspan="4">Synonyms: Triphenyl phosphate; TPP</td></tr>
<tr><td colspan="4">ASSESSMENT SUMMARY:</td></tr>
<tr><td rowspan="2"></td><td colspan="3">Concern Level</td></tr>
<tr><td>HIGH</td><td>MODERATE</td><td>LOW</td></tr>
<tr><td>Persistence</td><td></td><td></td><td>X</td></tr>
<tr><td>Bioconcentration</td><td></td><td></td><td>X</td></tr>
<tr><td>Cancer Health Hazard</td><td></td><td></td><td>X</td></tr>
<tr><td>Non-Cancer Health Hazard</td><td></td><td>X°</td><td></td></tr>
<tr><td>Aquatic Toxicity Hazard</td><td>X</td><td></td><td></td></tr>
<tr><td>Is the chemical predicted to be a PBT by PBT Profiler?</td><td colspan="3">No</td></tr>
<tr><td>Overall Hazard Concern</td><td colspan="3">Human Health Hazard: Moderate
Aquatic Hazard: High</td></tr>
</table>

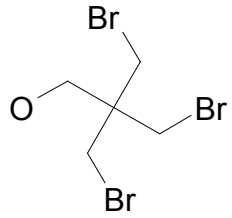
° Based on systemic effects and eye irritation.

Record ID: Triphenyl Phosphate	**CAS No.** 115-86-6
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	50.5 (M)
Boiling Point (deg C)	245 @ 11 mm Hg (M); 389 (E)
Vapor Pressure (mm Hg)	$6.3x10^{-6}$ (M)
Water Solubility (g/L)	$1.9x10^{-3}$ (M)
Log K_{ow}	4.59 (M)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC (atm-m^3/mole)	1.2×10^{-5} (M)
Soil Adsorption Coefficient – K_{oc}	2514-3561 (M)
Bioconcentration Factor – BCF	132-264 (Rainbow Trout); 218-1743 (Fathead Minnow) (M)
Persistence	
Experimental Biodeg Tests	93.8% removal as DOC in OECD 303A over 20 days; 50-100% removal within 8 days in river die-away; 83-84% over 28 days using MITI II; 10.3% removal in 40 days under anaerobic conditions in river sediment
Ultimate Biodeg Model	Weeks-months (E)
Primary Biodeg Model	Days (E)
BOD or COD	
Atmospheric Half-life	12 hours (E)
Hydrolysis Half-life	Half-life at 20 degrees C: 366 days@ pH 3; 406 days @ pH 7, <5 days @ pH 9 (M)
Volatilization Half-life for Model River	13 days (E)
Volatilization Half-life for Model Lake	152 days (E)
Removal in Sewage Treatment Plant	61% (E)
Ready Biodegradability	Ready biodegradable (M)
Byproducts	
Degradation Products	Diphenyl phosphate, phenol (M)
Metabolites	

Record ID: Triphenyl Phosphate	**CAS No.** 115-86-6
ECOTOXICITY:	
ECOSAR Class	Esters-phosphate
Comments	*** = based on geometric mean of experimental values**
Acute Toxicity	
Fish LC_{50}	96-h LC50, 0.870 mg/L (M)
Daphnid LC_{50}	48-h LC50, 1.2 mg/L (MC) 48-h LC50, 1.1 mg/L* (M)
Green Algae EC_{50}	96-h EC50, 2.0 mg/L (M)
Chronic Toxicity	
Fish ChV	0.140 mg/L (MC); 0.09 (F96/ACR10)(E)
Daphnid ChV	0.1 mg/L (D48/ACR10) (E)
Green Algae ChV	≥0.140 mg/L (E) < 0.600 mg/L (M) 0.5 mg/L (A96/ACR4) (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH
HEALTH EFFECTS:	
Absorption	Poor thru skin as neat solid, moderate thru skin in solution; moderate thru lungs and GI tract based on closely related analogs (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat, mouse, rabbit, oral, LD50 > 5000 mg/kg (M); Mammal, dermal, LD50 > 8000 mg/kg (MC); rabbit, dermal, LD50 > 7900 mg/kg (M)
Eye Irritation	Moderate; Mild eye irritation, rabbits (M, MC)
Skin Irritation	Low; Negative, rabbits (M)
Skin Sensitizer	Low; negative in guinea pigs (MC), very low incidence in humans (M)

Record ID: Triphenyl Phosphate	**CAS No.** 115-86-6
Reproductive Effects	Low; 91-112-d reproductive (incomplete)/developmental study, rats, diet, no reproductive effects, NOAEL = 690 mg/kg/day (1%) (M)
Developmental Effects	Low; 91-112-d reproductive/developmental study, rats, diet, no developmental effects, NOAEL = 690 mg/kg/day, maternal LOAEL = 690 mg/kg/day (1%) (M)
Immune System Effects	Low; 120-d repeated-dose study, rats, diet, no immune system effects, NOAEL = 700 mg/kg/day (1%) (M)
Neurotoxicity	Low; negative in delayed neurotoxicity studies in the hen at up to 10,000 mg/kg/day (oral, 6 dosing days) and in the cat at 700 mg/kg (subcutaneous, single dose) (M); 120-d repeated-dose neurotoxicity screening study, rats, diet, no neurobehavioral effects, NOAEL = 711 mg/kg/day (1.0%) (M)
Genotoxicity/Mutagenicity	Low; Negative in Ames assay and Negative in forward mutation assay, mouse lymphoma cells *in vitro*, with and without metabolic activation (M); Negative in mitotic gene conversion assay in *Saccharomyces cerevisiae* with and without activation (M)
Systemic Effects	Moderate; 35-d repeated-dose study (inadequate), rats, diet, increased relative liver weight at 0.5%, NOAEL = 0.1%; 120-d repeated-dose (neurotoxicity screening) study, rats, diet, decreased body weight gain without decreased food consumption, NOAEL = 161 mg/kg/day (0.25%), LOAEL = 345 mg/kg/day (1%); 21-d repeated-dose study (inadequate), rabbits, dermal, systemic effects (M)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.2 Tribromoneopentyl alcohol

Record ID: Tribromoneopentyl alcohol	**CAS No.** 36483-57-5
	**MW**: 324.84
	MF: $C_5H_9Br_3O$
	Physical Forms: **Neat:** Solid **As Formulated:**
	Use: Flame retardant, reactive
SMILES: OCC(CBr)(CBr)CBr	
Name: 1-Propanol, 2,2-dimethyl-, tribromo derivative (FRA-12)	
Synonyms: Tribromoneopentyl alcohol	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			***X***
Cancer Health Hazard		***X***	
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard		**X**	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

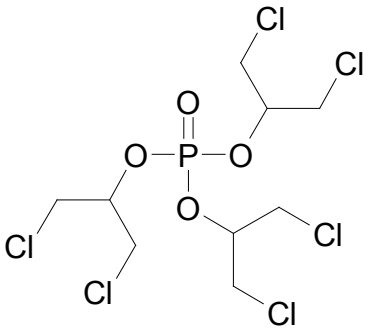
° Based on reproductive effects, developmental effects, neurotoxicity, genotoxicity/mutagenicity, systemic effects, eye irritation, and skin irritation.

Record ID: Tribromoneopentyl alcohol	**CAS No.** 36483-57-5
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	62-67 (M)
Boiling Point (deg C)	300 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	6.2×10^{-5} (E)
Water Solubility (g/L)	2 (M) 1.9 at 20.1 degrees C (MC)
Log K_{ow}	2.6 (MC)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	1.14×10^{-10} atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	22.9 (E)
Bioconcentration Factor – BCF	10.8 (E)
Persistence	
Experimental Biodeg Tests	2.5% CO2 evolution over 28 days in OECD 310 test (MC); 77% removal as DOC using OECD 302B in 36 days after a 10-day lag period (MC)
Ultimate Biodeg Model	Weeks-months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	25 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	2.55% (E)
Ready Biodegradability	Not ready biodegradable (MC)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound
Metabolites	

Record ID: Tribromoneopentyl alcohol	**CAS No.** 36483-57-5
ECOTOXICITY:	
ECOSAR Class	Haloalcohols
Acute Toxicity	
Fish LC_{50}	96-h LC50=32 mg/L (MC)
Daphnid LC_{50}	48-h EC50=64 mg/L (MC)
Green Algae EC_{50}	72-h EC50=28 mg/L (MC)
Chronic Toxicity	
Fish ChV	3.2 mg/L (F96/ACR 10) (E)
Daphnid ChV	6.4 mg/L (D48/ACR10) (E)
Green Algae ChV	7 mg/L (GA72/ACR4) (E)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Nil thru skin as neat material; moderate thru skin when in solution; good absorption expected thru lungs and GI tract (P)
CANCER HEALTH EFFECTS:	
Experimental data	Moderate by analogy to a closely related compound; 2-yr study, male/female, rats, mice, neoplasms in multiple organs (P)
OncoLogic Results	Moderate
Overall Hazard Concern for Carcinogenicity	MODERATE

Record ID: Tribromoneopentyl alcohol	**CAS No.** 36483-57-5
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD_{50} = 1630 to >2000 mg/kg (M,MC), effects on bladder (M); Rat dermal LD_{50} >2000 mg/kg (MC); Rat 7-h inhalation LC_{50} > 714 mg/m^3 (mixture, inadequate study) (M)
Eye Irritation	Moderate; Mild eye irritant in rabbits (M); moderate eye irritant in rabbits (MC)
Skin Irritation	Moderate; Mild skin irritant in rabbits 24 hr exposure (M) but not 4 hour exposure (MC)
Skin Sensitizer	Low; negative in mouse local lymph node assay (MC)
Reproductive Effects	Moderate by analogy to a closely related compound; repro/fertility study, mice, diet, 141, 274, 589 mg/kg/day, decreased fertility and litter size, increased gestation length, LOAEL = 141 mg/kg/day (P)
Developmental Effects	Moderate by analogy to a closely related compound; repro/fertility study, mice, diet, 141, 274, 589 mg/kg/day, decreased pup weight, NOAEL = 141 mg/kg/day (P)
Immune System Effects	
Neurotoxicity	Moderate based on bromo substituents (P)
Genotoxicity/Mutagenicity	Moderate; Positive, mutagenic in L5178Y mouse lymphoma cells with activation by rat S9 (MC); Positive, chromosomal aberrations, *in vitro* (MC); Positive, mouse micronucleus assay, females (MC); Positive, *Salmonella* with activation from hamster S9 (M, MC); Negative, *Salmonella* without activation or with activation by rat S9 (M, MC); Negative, yeast, mitotic gene conversion assay with or without activation (M)
Systemic Effects	Moderate; 30-d repeated-dose study, rats, oral, diet, 10, 30, 100, 300 mg/kg/day, kidney, ureter, bladder, blood changes, NOAEL = 30 mg/kg/day (M,P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.3 Tris(1,3-dichloro-2-propyl) Phosphate

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	**CAS No.** 13674-87-8
	**MW**: 430.91
	MF: $C_9H_{15}Cl_6O_4P$
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive
SMILES: ClCC(CCl)OP(=O)(OC(CCl)CCl)OC(CCl)CCl	
Name: 2-Propanol, 1,3-dichloro-, phosphate (3:1)	
Synonyms: Tris(1,3-dichloro-2-propyl) Phosphate, TDCPP; TDCP	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence		**X**	
Bioconcentration			***X***
Cancer Health Hazard		**X**	
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard		**X**	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

° Based on reproductive effects, developmental effects, genotoxicity/mutagenicity, systemic effects, eye irritation, and skin irritation.

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	**CAS No.** 13674-87-8
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	-58 (M)
Boiling Point (deg C)	236-237 @ 5 mm Hg (M); Slowly decomposes >200 (M)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	0.042 (M) 0.018 (MC)
Log K_{ow}	2.40 (M) 3.69 (MC)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC (atm-m^3/mol)	$2.61x10^{-9}$ (E)
Soil Adsorption Coefficient – K_{oc}	9222 (E)
Bioconcentration Factor – BCF	3-5 (Goldfish); 3-113 (Killifish) (M)
Persistence	
Experimental Biodeg Tests	0% CO_2 uptake over 28 days in OECD 301B test; 1% by BOD over 28 days in MITI test; 0% by 0_2 uptake over 28 days in OECD 302C test; 0-18.5% 0_2 uptake over 7-14 days in river die-away (M)
Ultimate Biodeg Model	Recalcitrant (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	7.1 hours (E)
Hydrolysis Half-life	>1 year @ pH 7
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	3% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound
Metabolites	

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	**CAS No.** 13674-87-8
ECOTOXICITY:	
ECOSAR Class	Esters - phosphate
Comments	* = based on geometric mean of experimental values
Acute Toxicity	
Fish LC_{50}	96-h LC50, 1.9 mg/L* (M,MC)
Daphnid LC_{50}	48-h LC50, 3.8 mg/L (E)
Green Algae EC_{50}	96-h EC50, 12.0 mg/L (M)
Chronic Toxicity	
Fish ChV	0.200 mg/L* (F96/ACR10) (E)
Daphnid ChV	0.400 mg/L (D48/ACR10) (E)
Green Algae ChV	6.0 mg/L (M)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Good absorption and reaction, all routes
CANCER HEALTH EFFECTS:	
Experimental data	2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased benign adrenal cortex tumors, testicular interstitial cell tumors, and hepatocellular adenomas at 20 and 80 mg/kg/day (M)
OncoLogic Results	Moderate
Overall Hazard Concern for Carcinogenicity	MODERATE
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Mouse oral LD_{50}= (male) 2670 & (female) 2250 mg/kg; Rat oral LD_{50} = 3160 mg/kg; Rabbit oral LD_{50} = 6800 mg/kg; Rabbit dermal (24-hr) LD_{50} >4640 mg/kg (no death, clinical signs or gross necropsy lesions)(M)
Eye Irritation	Moderate; Mild reversible conjunctival irritant or negative, rabbits (M)
Skin Irritation	Moderate; 4 Hrs: non-irritant; 24 hrs: mild skin irritant, rabbits (M)
Skin Sensitizer	Low; Negative in guinea pigs (MC); Uncertain concern for sensitization as substance is a potential alkylating agent (P)

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	**CAS No.** 13674-87-8
Reproductive Effects	Moderate; Male reproduction study, rabbits, gavage, 12-wk exposure, no effects on male fertility or spermatogenesis, NOAEL = 200 mg/kg/day (M); 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, anomalies of the testes and seminal vesicles, NOAEL = 5 mg/kg/day (M)
Developmental Effects	Moderate; Developmental toxicity study, gavage, rats, gd 6-15, 25, 100, 400 mg/kg/day, increased resorptions, decreased fetal viability, weight, and length, NOAEL = 100 mg/kg/day. Developmental toxicity study, gavage, rats, gd 7-19, 25, 50, 100, 200, 400 mg/kg/day, decreased fetal viability, NOAEL = 200 mg/kg/kday (M).
Immune System Effects	Low; Uncertain concern for immunotoxicity because substance is potentially an alkylating agent; Immunotoxicity assay, subcutaneous, mouse, 4 consecutive days, 0.25, 2.5, 25 mg/kg/day; lymphoid depletion of thymus, reduced responses to T-cell & B-cell antigens, NOAEL 0.25 mg/kg/day (M)
Neurotoxicity	Low; Acute delayed neurotoxicity study, hens, gavage, no significant inhibition of brain neurotoxic esterase (NTE) activity at 10,000 mg/kg; 90-d study, hens, gavage, no behavioral effects or histopathological changes indicative of neurotoxicity, NOAEL = 100 mg/kg/day; In developmental toxicity assay, rats, gavage gd 7-19, no adverse effect on postnatal neurobehavioral tests of sensory and motor function, NOAEL = 200 mg/kg/day (M)
Genotoxicity/ Mutagenicity	Moderate; Positive, mutagenicity, *Salmonella*, with metabolic activation; Negative, mutagenicity, mouse lymphoma cells with or without activation & hamster lung cells with activation, *in vitro*; Negative, sex-linked recessive lethal, *Drosophila in vivo* (M) Positive only with activation, chromosomal aberrations, *in vitro*, human lymphocytes (MC) & mouse lymphoma cells (M); Negative, chromosomal aberrations, *in vitro,* Chinese hamster ovary cells (MC); Negative, sister chromatid exchange, *in vitro*, cell line not reported (MC); Positive with or without activation, sister chromatid exchange, *in vitro,* mouse lymphoma cell; Negative, unscheduled DNA synthesis, in vivo, in rat hepatocytes (M, MC); Negative, chromosomal aberrations, in vivo, mice (M); Negative, micronucleus assay in vivo, mice (MC)

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	**CAS No.** 13674-87-8
Systemic Effects	Moderate; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased mortality, decreased body weight, anemia, anomalies of the liver, kidneys, testes, seminal vesicles, renal cortex, and adrenal cortex, LOAEL = 5 mg/kg/day. Inadequate 90-day dietary study, mice, 0.01, 0.04, 0.13, 0.42 and 1.33% in diet; increased mortality, decreased body weight, anemia, increased liver & kidney weight, liver histopathology; NOAEL= 0.01% dietary level (M)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.4 Proprietary A

Record ID: Proprietary A: Chloroalkyl phosphate (1)	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Chloroalkyl phosphate (1)	
Synonyms:	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence		**X**	
Bioconcentration			***X***
Cancer Health Hazard		**X**	
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard		**X**	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

° Based on reproductive effects, developmental effects, genotoxicity/mutagenicity, systemic effects, eye irritation, and skin irritation.

Record ID: Proprietary A: Chloroalkyl phosphate (1)	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	-58 (M)
Boiling Point (deg C)	236-237 @ 5 mm Hg (M); Slowly decomposes >200 (M)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	0.042 (M) 0.018 (MC)
Log K_{ow}	2.40 (M) 3.69 (MC)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC (atm-m^3/mol)	2.61×10^{-9} (E)
Soil Adsorption Coefficient – K_{oc}	9222 (E)
Bioconcentration Factor – BCF	3-5 (Goldfish); 3-113 (Killifish) (M)
Persistence	
Experimental Biodeg Tests	0% CO_2 uptake over 28 days in OECD 301B test; 1% by BOD over 28 days in MITI test; 0% by 0_2 uptake over 28 days in OECD 302C test; 0-18.5% 0_2 uptake over 7-14 days in river die-away (M)
Ultimate Biodeg Model	Recalcitrant (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	7.1 hours (E)
Hydrolysis Half-life	>1 year @ pH 7
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	3% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound
Metabolites	

Record ID: Proprietary A: Chloroalkyl phosphate (1)	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Esters - phosphate
Comments	* = based on geometric mean of experimental values
Acute Toxicity	
Fish LC_{50}	96-h LC50, 1.9 mg/L* (M,MC)
Daphnid LC_{50}	48-h LC50, 3.8 mg/L (E)
Green Algae EC_{50}	96-h EC50, 12.0 mg/L (M)
Chronic Toxicity	
Fish ChV	0.200 mg/L* (F96/ACR10) (E)
Daphnid ChV	0.400 mg/L (D48/ACR10) (E)
Green Algae ChV	6.0 mg/L (M)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Good absorption and reaction, all routes
CANCER HEALTH EFFECTS:	
Experimental data	2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased benign adrenal cortex tumors, testicular interstitial cell tumors, and hepatocellular adenomas at 20 and 80 mg/kg/day (M)
OncoLogic Results	Moderate
Overall Hazard Concern for Carcinogenicity	MODERATE
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Mouse oral LD_{50}= (male) 2670 & (female) 2250 mg/kg; Rat oral LD_{50} = 3160 mg/kg; Rabbit oral LD_{50} = 6800 mg/kg; Rabbit dermal (24-hr) LD_{50} >4640 mg/kg (no death, clinical signs or gross necropsy lesions)(M)
Eye Irritation	Moderate; Mild reversible conjunctival irritant or negative, rabbits (M)
Skin Irritation	Moderate; 4 Hrs: non-irritant; 24 hrs: mild skin irritant, rabbits (M)
Skin Sensitizer	Low; Negative in guinea pigs (MC); Uncertain concern for sensitization as substance is a potential alkylating agent (P)

Record ID: Proprietary A: Chloroalkyl phosphate (1)	**CAS No.**
Reproductive Effects	Moderate; Male reproduction study, rabbits, gavage, 12-wk exposure, no effects on male fertility or spermatogenesis, NOAEL = 200 mg/kg/day (M); 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, anomalies of the testes and seminal vesicles, NOAEL = 5 mg/kg/day (M)
Developmental Effects	Moderate; Developmental toxicity study, gavage, rats, gd 6-15, 25, 100, 400 mg/kg/day, increased resorptions, decreased fetal viability, weight, and length, NOAEL = 100 mg/kg/day. Developmental toxicity study, gavage, rats, gd 7-19, 25, 50, 100, 200, 400 mg/kg/day, decreased fetal viability, NOAEL = 200 mg/kg/kday (M).
Immune System Effects	Low; Uncertain concern for immunotoxicity because substance is potentially an alkylating agent; Immunotoxicity assay, subcutaneous, mouse, 4 consecutive days, 0.25, 2.5, 25 mg/kg/day; lymphoid depletion of thymus, reduced responses to T-cell & B-cell antigens, NOAEL 0.25 mg/kg/day (M)
Neurotoxicity	Low; Acute delayed neurotoxicity study, hens, gavage, no significant inhibition of brain neurotoxic esterase (NTE) activity at 10,000 mg/kg; 90-d study, hens, gavage, no behavioral effects or histopathological changes indicative of neurotoxicity, NOAEL = 100 mg/kg/day; In developmental toxicity assay, rats, gavage gd 7-19, no adverse effect on postnatal neurobehavioral tests of sensory and motor function, NOAEL = 200 mg/kg/day (M)
Genotoxicity/ Mutagenicity	Moderate; Positive, mutagenicity, Salmonella, with metabolic activation; Negative, mutagenicity, mouse lymphoma cells with or without activation & hamster lung cells with activation, in vitro; Negative, sex-linked recessive lethal, Drosophila in vivo (M) Positive only with activation, chromosomal aberrations, in vitro, human lymphocytes (MC) & mouse lymphoma cells (M); Negative, chromosomal aberrations, in vitro, Chinese hamster ovary cells (MC); Negative, sister chromatid exchange, in vitro, cell line not reported (MC); Positive with or without activation, sister chromatid exchange, in vitro, mouse lymphoma cell; Negative, unscheduled DNA synthesis, in vivo, in rat hepatocytes (M, MC); Negative, chromosomal aberrations, in vivo, mice (M); Negative, micronucleus assay in vivo, mice (MC)

Record ID: Proprietary A: Chloroalkyl phosphate (1)	**CAS No.**
Systemic Effects	Moderate; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased mortality, decreased body weight, anemia, anomalies of the liver, kidneys, testes, seminal vesicles, renal cortex, and adrenal cortex, LOAEL = 5 mg/kg/day. Inadequate 90-day dietary study, mice, 0.01, 0.04, 0.13, 0.42 and 1.33% in diet; increased mortality, decreased body weight, anemia, increased liver & kidney weight, liver histopathology; NOAEL= 0.01% dietary level (M)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.5 Proprietary B

Record ID: Proprietary B: Aryl phosphate	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:** Liquid
	Use: Flame retardant, additive
SMILES:	
Name: Aryl phosphate	
Synonyms:	

ASSESSMENT SUMMARY:			
	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			***X***
Bioconcentration		***X***	
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

° Based on reproductive effects, developmental effects, neurotoxicity, systemic effects, and eye irritation.

Record ID: Proprietary B: Aryl phosphate	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	90 (E)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	$<10^{-6}$ (E)
Log K_{ow}	6.16 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$7.74x10^{-8}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	$2.6x10^4$ (E)
Bioconcentration Factor – BCF	1820 (E)
Persistence	
Experimental Biodeg Tests	46% ThOD after 28 days in OECD 301F (MC)
Ultimate Biodeg Model	Weeks -months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	9.3 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	605 days (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	93% (E)
Ready Biodegradability	Not ready biodegradable (MC)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound
Metabolites	

Record ID: Proprietary B: Aryl phosphate	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)
Daphnid LC_{50}	48-h LC50, NES (E)
Green Algae EC_{50}	96-h EC50, NES (E)
Chronic Toxicity	
Fish ChV	NES (E)
Daphnid ChV	NES (E)
Green Algae ChV	NES (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity and only when 1 or 2 isopropyls are present)
HEALTH EFFECTS:	
Absorption	Nil thru skin as neat solid; poor thru skin when in solution; poor thru lungs and GI tract by analogy to closely related compounds (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary B: Aryl phosphate	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low in mixtures; Rat oral LD_{50} >5000 mg/kg (no deaths), >20,000 mg/kg (4/10 deaths); Rat 1-hr inhalation LC_{50} > 200 mg/L; Rat dermal LD_0 > 2000 mg/kg (no deaths)(M)
Eye Irritation	Moderate in mixtures; Rabbits, very slight eye irritation (M)
Skin Irritation	Low in mixtures; Not irritating to intact or abraded skin in rabbits (M)
Skin Sensitizer	Low by analogy to a closely related compound (P)
Reproductive Effects	Preliminary results of an unfinished 39-41-day combined subchronic plus reproductive/developmental toxicity screening test suggest that the reproductive hazard may be moderate, rat, oral gavage, ovarian weight effect at ≥25 mg/kg/day, epididymal weight effect and reduced fertility at 100 and 400 mg/kg/day (MC)
Developmental Effects	Preliminary results of an unfinished 39-41-day combined subchronic plus reproductive/developmental toxicity screening test suggests the developmental hazard may be moderate; rat, oral gavage, reduced pre- and post-natal survival at 400 mg/kg/day (MC)
Immune System Effects	
Neurotoxicity	Moderate in mixtures; acute delayed neurotoxicity assay, hens, oral gavage, NOAEL = 12 mg/kg/day for neurotoxic esterase (NTE) inhibition, LOAEL = 1000 mg/kg/day; delayed oral neurotoxicity, hens, 2 oral treatments 3 weeks apart, transient dose-related gait impairment (LOAEL = 12 mg/kg/day), but no neurohistopathology at doses as high as 11,700 mg/kg/day (M); Also by analogy to closely related compounds and professional judgment; neurotoxicity study, hens, oral gavage, 3, 5, 7, 9 g/kg, ataxia, neuropathological lesions, LOAEL = 3000 mg/kg; neurotoxicity study, hens, oral gavage, 10, 20, 90, 270 mg/kg/day, ataxia, nerve degeneration, NOAEL = 20 mg/kg/day; NTE inhibition (M,P)
Genotoxicity/Mutagenicity	Low by analogy to a closely related compound; Negative, Ames assay (P)
Systemic Effects	Moderate in mixture (liver effects); 28-d repeated-dose study (inadequate), rats, diet, 0.1%, 0.5%, 1.0%, liver effects all doses, LOAEL = 0.1% (M); Preliminary results of an unfinished a 39-41-day combined subchronic toxicity with reproductive/developmental screening test suggest that there may be a moderate hazard for subchronic toxicity (adrenal and liver effects), rat, oral gavage, adrenal weight effect in females, LOAEL = 25 mg/kg/day (MC)

Record ID: Proprietary B: Aryl phosphate	**CAS No.**
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.6 Proprietary C

Record ID: Proprietary C: Chloroalkyl phosphate (2)	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:** Liquid
	Use: Flame retardant, additive
SMILES:	
Name: Chloroalkyl phosphate (2)	
Synonyms:	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence		**X**	
Bioconcentration			***X***
Cancer Health Hazard		***X***	
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard		**X**	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

° Based on reproductive effects, developmental effects, systemic effects, eye irritation, skin irritation, and skin sensitizer.

Record ID: Proprietary C: Chloroalkyl phosphate (2)	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (MC)
Water Solubility (g/L)	0.23 (MC)
Log K_{ow}	2.83 (MC)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$2.74x10^{-14}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	$1.1x10^4$ (MC); $6.07x10^6$ (E)
Bioconcentration Factor – BCF	6.64 (E)
Persistence	
Experimental Biodeg Tests	37% oxygen uptake after 28 days in OECD 302C (MC); 5% degradation in modified Sturm test, 28 days (MC); 8-15% inhibition to activated sludge (MC)
Ultimate Biodeg Model	Recalcitrant (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	1.6 hours (E)
Hydrolysis Half-life	Half-life is greater than 1 year (MC)
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	44.7% (E)
Ready Biodegradability	Not ready biodegradable (MC)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound
Metabolites	

Record ID: Proprietary C: Chloroalkyl phosphate (2)	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, 9.6 mg/L (E) 96-h LC50, 52.2 mg/L (MC)
Daphnid LC_{50}	48-h EC50, 30.0 mg/L (E) 48-h EC50, 41.9 mg/L (MC)
Green Algae EC_{50}	96-h EC50, 1.5 mg/L (E) 96-h EC50 (growth rate inhibition), 38.5 mg/L (MC) 96-h EC50 (growth inhibition), 20.1 mg/L (MC)
Chronic Toxicity	
Fish ChV	1.0 mg/L (E)
Daphnid ChV	3.0 mg/L, (E) 23-d EC50 (parental mortality), 7.31 mg/L (MC) LOEC (impaired reproduction), > 3.68 mg/L (MC) NOEC (impaired reproduction), ≥ 3.68 mg/L (MC)
Green Algae ChV	1.2 mg/L (E)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Poor absorption via all routes (P)
CANCER HEALTH EFFECTS:	
Experimental data	Moderate by analogy to a closely related compound; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased benign adrenal cortex tumors and hepatocellular adenomas at 20 and 80 mg/kg/day (P)
OncoLogic Results	Low-moderate (E)
Overall Hazard Concern for Carcinogenicity	MODERATE
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD_{50} between 2000 and 5000 mg/kg (M), >2000 mg/kg (MC); Rat inhalation LC_{50} >1.65 mg/L (no death) (MC); Rat dermal LD_{50} > 2000 mg/kg (no deaths or clinical signs)(M, MC)
Eye Irritation	Moderate; Slight eye (conjunctival) irritation (M, MC)
Skin Irritation	Moderate, rabbits; No skin irritation (M); slight irritation (erythema) (MC); mild irritation (erythema, edema) (MC)

Record ID: Proprietary C: Chloroalkyl phosphate (2)	**CAS No.**
Skin Sensitizer	Moderate; guinea pig, no sensitization (M), mild sensitization (MC)
Reproductive Effects	A 4-wk oral gavage study in rats reported no histopathology of reproductive organs in either sex at a NOAEL of 600 mg/kg/day, but the study duration was short (MC); Moderate by analogy to a closely related compound; 12-wk male reproduction study, rabbits, gavage, no effects on male fertility or spermatogenesis, NOAEL = 200 mg/kg/day; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, anomalies of the testes and seminal vesicles, NOAEL = 5 mg/kg/day (P)
Developmental Effects	Moderate by analogy to closely related compound; Developmental toxicity study on one analog, gavage, rats, gd 6-15, 25, 100, 400 mg/kg/day, increased resorptions, decreased fetal viability, weight, and length, fetal NOAEL = 100 mg/kg/day (P); Developmental toxicity study on another analog, gavage, rats, 15, 50, 150, 500 mg/kg/day, maternal deaths at 150 mg/kg/day, maternal NOAEL = 50 mg/kg/day, fetal NOAEL = 15 mg/kg/day (P)
Immune System Effects	
Neurotoxicity	Low, neurotoxicity screening battery after 4-week oral gavage, rats, no behavioral effects or neurohistopathology, NOAEL = 600 mg/kg/day (MC). Also by analogy to a closely related compound; Acute study, hens, gavage, delayed neurotoxicity, no inhibition of brain neurotoxic esterase (NTE) activity, NOAEL = 10,000 mg/kg; 90-d study, hens, gavage, no behavioral effects or histopathological changes indicative of neurotoxicity, NOAEL = 100 mg/kg/day (P)
Genotoxicity/Mutagenicity	Low, Negative, mutagenicity in mouse lymphoma (M, MC) and Ames test (MC); Negative, chromosomal aberrations *in vitro* (human lymphocytes) (MC); Negative, bone marrow micronucleus assay in mice (oral gavage) (MC) Moderate for genotoxic effects other than mutagenicity by analogy to closely related compounds: Positive, chromosomal aberrations, *in vitro*, human lymphocytes; Positive, rat dominant lethal assay (P);

Record ID: Proprietary C: Chloroalkyl phosphate (2)	**CAS No.**
Systemic Effects	Moderate, 4-week oral gavage study, rats (liver effects), NOAEL = 15 mg/kg,day, LOAEL = 150 mg/kg/day (MC); Also by analogy to a closely related compound; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased mortality, decreased body weight, anomalies of the liver, kidneys, testes, seminal vesicles, renal cortex, and adrenal cortex, NOAEL = 5 mg/kg/day (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.7 Proprietary D

Record ID: Proprietary D: Reactive brominated flame retardant	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:** Liquid
	Use: Flame retardant, reactive
SMILES:	
Name: Reactive brominated flame retardant	
Synonyms:	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			***X***△
Bioconcentration			***X***
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X**°	
Aquatic Toxicity Hazard		**X**	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

△ Likely brominated hydrolysis product is expected to be persistent.

° Based on neurotoxicity, systemic effects, eye irritation, and skin sensitizer.

Record ID: Proprietary D: Reactive brominated flame retardant	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	0.007 to 0.15 (E)
Log K_{ow}	3.83 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$2.23x10^{-21}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	10 (E)
Bioconcentration Factor – BCF	39 (E)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	4.2 hours (E)
Hydrolysis Half-life	19 hrs @ pH 8; 7 days @ pH 7 (E)
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	23% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	Brominated hydrolysis product (P)
Metabolites	

Record ID: Proprietary D: Reactive brominated flame retardant	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phthalate
Acute Toxicity	
Fish LC_{50}	96-h LC50, ≤ 67.0 mg/L (E)
Daphnid LC_{50}	48-h LC50, ≤ 280.0 mg/L (E)
Green Algae EC_{50}	96-h EC50, ≤ 5.4 mg/L (E)
Chronic Toxicity	
Fish ChV	≤ 7.0 mg/L (E)
Daphnid ChV	≤ 30.0 mg/L (E)
Green Algae ChV	≤ 4.2 mg/L (E)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Poor all routes (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary D: Reactive brominated flame retardant	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD_{50} >10,000 mg/kg (no deaths); Rabbit dermal LD_{50} >20,000 mg/kg (no deaths); Rat 1-hr inhalation LC_{50} >0.008 mg/L (no deaths) (M); Low by analogy to a closely related compound; Rat oral LD_{50} = 2874 (P)
Eye Irritation	Moderate, mild reversible conjunctival irritant or not an eye irritant in rabbits (M)
Skin Irritation	Low, not an irritant to intact skin, mild reversible irritation of abraded skin in rabbits (M)
Skin Sensitizer	Moderate by analogy to a closely related compound (P)
Reproductive Effects	
Developmental Effects	
Immune System Effects	
Neurotoxicity	Moderate by analogy to a closely related compound: Acute oral study, rats, brain hemorrhages (P)
Genotoxicity/Mutagenicity	Low, Negative in Ames assay with or without metabolic activation (M); Low also by analogy to a closely related compound; Negative in Ames assay (P)
Systemic Effects	Moderate by analogy to closely related compounds: 28-d, rats, oral, 160, 400, 1000 mg/kg/day, renal effects at all doses; 21-d repeated-dose study, rats, inhalation, 2-8 mg/L, adrenal, thyroid, lung, and liver effects; 28-d repeated-dose study, rabbits, dermal, 5000 mg/kg, kidney, liver, blood effects (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.8 Proprietary E

Record ID: Proprietary E: Tetrabromophthalate diol diester			**CAS No.**
			MW:
			MF:
			Physical Forms: **Neat:** Solid **As Formulated:** Liquid
			Use: Flame retardant, additive
SMILES:			
Name: Tetrabromophthalate diol diester			
Synonyms:			
ASSESSMENT SUMMARY:			
	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			***X***△
Bioconcentration			***X***
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X**°	
Aquatic Toxicity Hazard			
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard:**		

△ Likely brominated hydrolysis product is expected to be persistent.
° Based on systemic effects.

Record ID: Proprietary E: Tetrabromophthalate diol diester	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	0.002 (E)
Log K_{ow}	5.57 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$<10^{-8}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	27,000 (E)
Bioconcentration Factor – BCF	3,903 (E); Low, hydrolyzes
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Recalcitrant (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	3.2 hours (E)
Hydrolysis Half-life	8 days @ p-H 7; 19 hours @ pH 8 (E)
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	89% (E)
Ready Biodegradability	Not Ready Biodegradable (E)
Byproducts	
Degradation Products	Tetrabromophthalate by hydrolysis (P)
Metabolites	

Record ID: Proprietary E: Tetrabromophthalate diol diester	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phthalate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)
Daphnid LC_{50}	48-h LC50, NES (E)
Green Algae EC_{50}	96-h EC50, NES (E)
Chronic Toxicity	
Fish ChV	0.040 or NES (E)
Daphnid ChV	0.030 or NES (E)
Green Algae ChV	0.100 or NES (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity only)
HEALTH EFFECTS:	
Absorption	Absorption of LMW fraction is expected to be poor by all routes based on physicochemical properties (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Cannot be run in OncoLogic
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary E: Tetrabromophthalate diol diester	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	
Eye/Skin Irritation	
Skin Sensitizer	
Reproductive Effects	
Developmental Effects	
Immune System Effects	
Neurotoxicity	
Genotoxicity/Mutagenicity	
Systemic Effects	Moderate by analogy to closely related compounds; kidney toxicity, NOAEL = 400 mg/kg (M); liver toxicity based on brominated phenyl moiety (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.9 Proprietary F

Record ID: Proprietary F: Halogenated aryl ester	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Halogenated aryl ester	
Synonyms:	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			**X**△
Bioconcentration			**X**
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X**°	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Low**		

△ Likely halogenated degradation product is expected to be persistent.
° Based on reproductive effects, developmental effects, and systemic effects.

Record ID: Proprietary F: Halogenated aryl ester	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<1x10^{-6}$ (E)
Water Solubility (g/L)	0.002 (MC)
Log Kow	8.75 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	7.05×10^{-6} atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	>28,840 (MC)
Bioconcentration Factor – BCF	1.7-6.2 (MC)
Persistence	
Experimental Biodeg Tests	Half-life of 3.5 days in water shake flask die-away test, 8.5 days in sediment (MC); 6% biodegradation after 28 days in closed bottle test (MC)
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	12 hours (E)
Hydrolysis Half-life	>1 year @ pH 4, 7, and 9 (MC)
Volatilization Half-life for Model River	8 days (E)
Volatilization Half-life for Model Lake	98 days (E)
Removal in Sewage Treatment Plant	90% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	Halogenated aryl acid
Metabolites	

Record ID: Proprietary F: Halogenated aryl ester	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Esters
Acute Toxicity	
Fish LC_{50}	96 hr NOEC, NES (No effects at saturation) (MC)
Daphnid LC_{50}	24 hr EC50, 1.2 mg/L; 48 hr EC50, 0.42 mg/L (MC)
Green Algae EC_{50}	96 hr EC50, NES (MC)
Chronic Toxicity	
Fish ChV	NES (E)
Daphnid ChV	0.04 (D48/ACR10) (E)
Green Algae ChV	NES (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH
HEALTH EFFECTS:	
Absorption	Poor absorption via all routes (P)
CANCER HEALTH EFFECTS:	
Experimental data	Uncertain by analogy to a closely related chemical classes (P)
OncoLogic Results	
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary F: Halogenated aryl ester	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD50 >2000 mg/kg (M)
Eye Irritation	
Skin Irritation	
Skin Sensitizer	
Reproductive Effects	Moderate by analogy to a closely related compound (P)
Developmental Effects	Moderate by analogy to a closely related compound (P)
Immune System Effects	
Neurotoxicity	
Genotoxicity/Mutagenicity	
Systemic Effects	Moderate concern for liver effects by analogy to a closely related compound (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.10 Proprietary G

Record ID: Proprietary G: Triaryl phosphate, isopropylated	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:** Liquid
	Use: Flame retardant, additive
SMILES:	
Name: Triaryl phosphate, isopropylated	
Synonyms:	

ASSESSMENT SUMMARY:			
	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			***X***
Bioconcentration		***X***	
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

° Based on reproductive effects, developmental effects, neurotoxicity, systemic effects, and eye irritation.

Record ID: Proprietary G: Triaryl phosphate, isopropylated	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	90 (E)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	$<10^{-6}$ (E)
Log K_{ow}	6.16 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$7.74x10^{-8}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	$2.6x10^4$ (E)
Bioconcentration Factor – BCF	1820 (E)
Persistence	
Experimental Biodeg Tests	46% ThOD after 28 days in OECD 301F (MC)
Ultimate Biodeg Model	Weeks -months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	9.3 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	605 days (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	93% (E)
Ready Biodegradability	Not ready biodegradable (MC)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound
Metabolites	

Record ID: Proprietary G: Triaryl phosphate, isopropylated	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)
Daphnid LC_{50}	48-h LC50, NES (E)
Green Algae EC_{50}	96-h EC50, NES (E)
Chronic Toxicity	
Fish ChV	NES (E)
Daphnid ChV	NES (E)
Green Algae ChV	NES (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity and only when 1 or 2 isopropyls are present)
HEALTH EFFECTS:	
Absorption	Nil thru skin as neat solid; poor thru skin when in solution; poor thru lungs and GI tract by analogy to closely related compounds (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary G: Triaryl phosphate, isopropylated	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low in mixtures; Rat oral LD_{50} >5000 mg/kg (no deaths), >20,000 mg/kg (4/10 deaths); Rat 1-hr inhalation LC_{50} > 200 mg/L; Rat dermal LD_0 > 2000 mg/kg (no deaths)(M)
Eye Irritation	Moderate in mixtures; Rabbits, very slight eye irritation (M)
Skin Irritation	Low in mixtures; Not irritating to intact or abraded skin in rabbits (M)
Skin Sensitizer	Low by analogy to a closely related compound (P)
Reproductive Effects	Preliminary results of an unfinished 39-41-day combined subchronic plus reproductive/developmental toxicity screening test suggest that the reproductive hazard may be moderate, rat, oral gavage, ovarian weight effect at ≥25 mg/kg/day, epididymal weight effect and reduced fertility at 100 and 400 mg/kg/day (MC)
Developmental Effects	Preliminary results of an unfinished 39-41-day combined subchronic plus reproductive/developmental toxicity screening test suggests the developmental hazard may be moderate; rat, oral gavage, reduced pre- and post-natal survival at 400 mg/kg/day (MC)
Immune System Effects	
Neurotoxicity	Moderate in mixtures; acute delayed neurotoxicity assay, hens, oral gavage, NOAEL = 12 mg/kg/day for neurotoxic esterase (NTE) inhibition, LOAEL = 1000 mg/kg/day; delayed oral neurotoxicity, hens, 2 oral treatments 3 weeks apart, transient dose-related gait impairment (LOAEL = 12 mg/kg/day), but no neurohistopathology at doses as high as 11,700 mg/kg/day (M); Also by analogy to closely related compounds and professional judgment; neurotoxicity study, hens, oral gavage, 3, 5, 7, 9 g/kg, ataxia, neuropathological lesions, LOAEL = 3000 mg/kg; neurotoxicity study, hens, oral gavage, 10, 20, 90, 270 mg/kg/day, ataxia, nerve degeneration, NOAEL = 20 mg/kg/day; NTE inhibition (M,P)
Genotoxicity/Mutagenicity	Low by analogy to a closely related compound; Negative, Ames assay (P)
Systemic Effects	Moderate in mixture (liver effects); 28-d repeated-dose study (inadequate), rats, diet, 0.1%, 0.5%, 1.0%, liver effects all doses, LOAEL = 0.1% (M); Preliminary results of an unfinished a 39-41-day combined subchronic toxicity with reproductive/developmental screening test suggest that there may be a moderate hazard for subchronic toxicity (adrenal and liver effects), rat, oral gavage, adrenal weight effect in females, LOAEL = 25 mg/kg/day (MC)

Record ID: Proprietary G: Triaryl phosphate, isopropylated	**CAS No.**
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.11 Proprietary H

Record ID: Proprietary H: Halogenated aryl ester	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Halogenated aryl ester	
Synonyms:	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			**X**△
Bioconcentration			**X**
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X**°	
Aquatic Toxicity Hazard-	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Low**		

△ Likely halogenated degradation product is expected to be persistent.
° Based on reproductive effects, developmental effects, and systemic effects.

Record ID: Proprietary H: Halogenated aryl ester	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<1x10^{-6}$ (E)
Water Solubility (g/L)	0.002 (MC)
Log K_{ow}	12.0 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$3.08x10^{-7}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	>28,840 (MC)
Bioconcentration Factor – BCF	1.7-6.2 (MC)
Persistence	
Experimental Biodeg Tests	Half-life of 3.5 days in water shake flask die-away test, 8.5 days in sediment (MC); 6% biodegradation after 28 days in closed bottle test (MC)
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	6 hours (E)
Hydrolysis Half-life	>1 year @ pH 4, 7, and 9 (MC)
Volatilization Half-life for Model River	211 days (E)
Volatilization Half-life for Model Lake	2310 days (E)
Removal in Sewage Treatment Plant	90% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	Halogenated aryl acid
Metabolites	

Record ID: Proprietary H: Halogenated aryl ester	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Esters
Acute Toxicity	
Fish LC_{50}	96 hr NOEC, NES (No effects at saturation) (MC)
Daphnid LC_{50}	24 hr EC50, 1.2 mg/L; 48 hr EC50, 0.42 mg/L (MC)
Green Algae EC_{50}	96 hr EC50, NES (MC)
Chronic Toxicity	
Fish ChV	NES (E)
Daphnid ChV	0.04 (D48/ACR10) (E)
Green Algae ChV	NES (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH
HEALTH EFFECTS:	
Absorption	Poor absorption via all routes (P)
CANCER HEALTH EFFECTS:	
Experimental data	Uncertain by analogy to a closely related chemical classes (P)
OncoLogic Results	
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary H: Halogenated aryl ester	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD50 >2000 mg/kg (M)
Eye Irritation	
Skin Irritation	
Skin Sensitizer	
Reproductive Effects	Moderate by analogy to a closely related compound (P)
Developmental Effects	Moderate by analogy to a closely related compound (P)
Immune System Effects	
Neurotoxicity	
Genotoxicity/Mutagenicity	
Systemic Effects	Moderate concern for liver effects by analogy to a closely related compound (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.12 Proprietary I

Record ID: Proprietary I: Organic phosphate ester	**CAS No**.
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Organic phosphate ester	
Synonyms:	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence	**X**		
Bioconcentration			**X**
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**Yes**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

° Based on systemic effects and eye irritation.

Record ID: Proprietary I: Organic phosphate ester	**CAS No**.
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>300 (MC)
Boiling Point Pressure (mm Hg)	760 (MC)
Vapor Pressure (mm Hg)	$<10^{-6}$ (MC)
Water Solubility (g/L)	$8x10^{-4}$ (MC,P)
Log K_{ow}	6.89 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$4.89x10^{-14}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	$5.0x10^7$ (E)
Bioconcentration Factor – BCF	245 (MC)
Persistence	
Experimental Biodeg Tests	2.3% degradation after 28 days MITI-II (MC); 30% in 28 days and 52% in 140 days - closed bottle test (MC)
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Days (E)
BOD or COD	
Atmospheric Half-life	2.1 hours (E)
Hydrolysis Half-life	Half-life of 20 days at pH 9 and 25 deg C (MC)
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	94% (E)
Ready Biodegradability	Not Ready Biodegradable (MC)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound

Record ID: Proprietary I: Organic phosphate ester	**CAS No**.
Metabolites	
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E) 96-h LC50, 0.205 mg/L (MC)
Daphnid LC_{50}	48-h LC50, NES (E) 48-h LC50, > 0.846 mg/L (MC)
Green Algae EC_{50}	96-h EC50, NES (E)
Chronic Toxicity	
Fish ChV	0.200 or NES (E) LOEC (reduced larval survival and growth), 0.088 mg/L (MC)
Daphnid ChV	0.070 or NES (E) LOEC (reduced reproduction and growth), 0.147 mg/L (MC)
Green Algae ChV	0.140 or NES (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity only)
HEALTH EFFECTS:	
Absorption	Poor all routes by analogy to closely related compounds and physicochemical properties (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary I: Organic phosphate ester	**CAS No**.
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; rat oral LD_{50} > 5 g/kg; rabbit dermal LD_{50} > 5 g/kg; LC_{50}>1.55 mg/L (MC)
Eye Irritation	Moderate; mild and transient eye irritation, rabbits; no eye irritation, rabbits (MC)
Skin Irritation	Low; no skin irritation in rabbits (MC)
Skin Sensitizer	Low; no skin sensitization in guinea pigs (MC)
Reproductive Effects	Low; NOAEL>1000 mg/kg/day in reproductive/developmental screening test in rats (MC)
Developmental Effects	Low; NOAEL>1000 mg/kg/day in reproductive/developmental screening test in rats (MC)
Immune System Effects	
Neurotoxicity	Low by analogy to a closely related compound; 42-d neurotoxicity test, hens, NOAEL = 5 g/kg/day (P)
Genotoxicity/Mutagenicity	Low; Negative, mouse micronucleus assay, *in vivo*, i.p.; Negative, chromosomal aberrations *in vitro*; Negative Ames assay, *Salmonella* and *E. coli*; Negative mouse lymphoma assay (MC)
Systemic Effects	Moderate by analogy to a closely related compound; 28-d repeated-dose study, rat, oral gavage, slight liver toxicity, NOAEL = 300 mg/kg/day, LOAEL = 1000 mg/kg/day (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.13 Proprietary J

Record ID: Proprietary J: Aryl phosphate	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Aryl phosphate	
Synonyms:	

ASSESSMENT SUMMARY:

	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			***X***
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

° Based on systemic effects and eye irritation.

Record ID: Proprietary J: Aryl phosphate	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	-21 (M)
Boiling Point (deg C)	425 (M)
Boiling Point Pressure (mm Hg)	760 (M)
Vapor Pressure (mm Hg)	$1.4x10^{-6}$ (M)
Water Solubility (g/L)	0.0032 (M)
Log K_{ow}	5.12 (M)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$8.48x10^{-7}$ atm-m^3/mole (M)
Soil Adsorption Coefficient – K_{oc}	$3.7x10^4$ (E)
Bioconcentration Factor – BCF	290 (E)
Persistence	
Experimental Biodeg Tests	43-90% CO2 evolution in 28 days with activated sludge inoculum; 50% removal in 11 days in river die away; half life of 0.44 days in pond water and 39 days in pond sediment
Ultimate Biodeg Model	Weeks-months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	8.2 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	54 days (E)
Volatilization Half-life for Model Lake	594 days (E)
Removal in Sewage Treatment Plant	81.2% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound
Metabolites	

Record ID: Proprietary J: Aryl phosphate	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)
Daphnid LC_{50}	48-h LC50, NES (E)
Green Algae EC_{50}	96-h EC50, 0.020 mg/L or NES (E)
Chronic Toxicity	
Fish ChV	0.003 mg/L (E)
Daphnid ChV	0.002 mg/L (E)
Green Algae ChV	0.020 mg/L (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity only)
HEALTH EFFECTS:	
Absorption	Nil thru skin as neat solid; poor thru skin when in solution; poor thru lungs and GI tract by analogy to closely related compounds (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary J: Aryl phosphate	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD_{50} > 5000 mg/kg; Rat dermal LD_{50} > 2000 mg/kg (M)
Eye Irritation	Low; Rabbits, no eye irritation (M)
Skin Irritation	Moderate; Rabbits, mild skin irritation (M)
Skin Sensitizer	Low by analogy to a closely related compound (P)
Reproductive Effects	Low, 90-day oral toxicity (diet), rats, no effect on histopathology or weights of reproductive organs in males or females, NOAEL = 1600 ppm (M)
Developmental Effects	
Immune System Effects	
Neurotoxicity	Low, delayed neurotoxicity; 5-d study, hens, oral gavage, 5000 mg/kg/day, no evidence of delayed neurotoxicity; 90-day oral toxicity (diet), rats, no neurohistopathology in males or females, NOAEL = 1600 ppm (M); Also by analogy to a closely related compound (P)
Genotoxicity/Mutagenicity	Studies on poorly defined mixtures suggest negative results for mutagenicity (*Salmonella typhimurium, Saccharomyces cerevisiae*, mouse lymphoma cells), chromosomal aberration *in vitro* (mouse lymphoma cells) and sister chromatid exchange *in vitro* (mouse lymphoma cells) (M)
Systemic Effects	Moderate, based on studies identifying liver as potential target organ. 90-day oral toxicity (diet), rats, at 1600 ppm (125 mg/kg/day), increased absolute and relative liver weights (both sexes) and adrenal weights (females), no histopathological lesions, but not tested at limit dose, NOAEL = 400 ppm, LOAEL = 1600 ppm (M); Also by analogy to closely related compounds (liver effects); 28-d repeated-dose study (inadequate), rats, diet, increased relative liver weight (no histopathology data available) at 0.5%, NOAEL = 0.1% (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.14 Proprietary K

Record ID: Proprietary K: Aryl phosphate	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Aryl phosphate	
Synonyms:	

ASSESSMENT SUMMARY:			
	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			***X***
Bioconcentration			***X***
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard			**X**
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Low**		

° Based on systemic effects.

Record ID: Proprietary K: Aryl phosphate	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	90 (E)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	$<10^{-6}$ (E)
Log K_{ow}	8.52 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$2.65x10^{-7}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	$2.7x10^{5}$ (E)
Bioconcentration Factor – BCF	89 (E)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	9.7 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	193 days (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	94% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	Degradation products are expected to be less persistent than the parent compound
Metabolites	

Record ID: Proprietary K: Aryl phosphate	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)
Daphnid LC_{50}	48-h LC50, NES (E)
Green Algae EC_{50}	96-h EC50, NES (E)
Chronic Toxicity	
Fish ChV	NES (E)
Daphnid ChV	NES (E)
Green Algae ChV	NES (E)
Overall Hazard Concern for Aquatic Toxicity	LOW
HEALTH EFFECTS:	
Absorption	Nil thru skin as neat solid; poor thru skin when in solution; poor thru lungs and GI tract by analogy to closely related compounds (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary K: Aryl phosphate	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	
Eye/Skin Irritation	
Skin Sensitizer	Low by analogy to a closely related compound (P)
Reproductive Effects	
Developmental Effects	
Immune System Effects	
Neurotoxicity	Low by analogy to a closely related compound (P)
Genotoxicity/Mutagenicity	
Systemic Effects	Moderate by analogy to closely related compounds (liver effects); 28-d repeated-dose study (inadequate), rats, diet, liver effects at 0.5%, NOAEL = 0.1% (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.15 Proprietary L

Record ID: Proprietary L: Aryl phosphate	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Aryl phosphate	
Synonyms:	

ASSESSMENT SUMMARY:			
	Concern Level		
	HIGH	**MODERATE**	**LOW**
Persistence			***X***
Bioconcentration			***X***
Cancer Health Hazard			***X***
Non-Cancer Health Hazard		**X°**	
Aquatic Toxicity Hazard			**X**
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Low**		

° Based on systemic effects.

Record ID: Proprietary L: Aryl phosphate	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	90 (E)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	$<10^{-6}$ (E)
Log K_{ow}	10.43 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC (atm-m^3/mole)	$6.85x10^{-7}$ (E)
Soil Adsorption Coefficient – K_{oc}	$1.9x10^{6}$ (E)
Bioconcentration Factor – BCF	3.1 (E)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Recalcitrant (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	8.8 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	79 days (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	94% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary L: Aryl phosphate	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Esters-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)
Daphnid LC_{50}	48-h LC50, NES (E)
Green Algae EC_{50}	96-h EC50, NES (E)
Chronic Toxicity	
Fish ChV	NES (E)
Daphnid ChV	NES (E)
Green Algae ChV	NES (E)
Overall Hazard Concern for Aquatic Toxicity	LOW
HEALTH EFFECTS:	
Absorption	Nil thru skin as neat solid, poor thru skin in solution; poor thru lungs and GI tract, based on closely related analogs
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary L: Aryl phosphate	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	
Eye Irritation	
Skin Irritation	
Skin Sensitizer	Low, concern for sensitization by analogy to closely related compounds (P)
Reproductive Effects	
Developmental Effects	
Immune System Effects	
Neurotoxicity	Low; Not neurotoxic by analogy to a closely related compound which yielded negative results in all reliable oral assays for delayed acute neurotoxicity in hens and subchronic neurobehavioral assays in rats (M); Proprietary L lacks structural motifs associated with neurotoxicity (P)
Genotoxicity/ Mutagenicity	
Systemic Effects	Moderate, systemic effects by analogy to closely related compounds, including 28-d repeated-dose study (inadequate), rats, diet, liver effects at 0.5%, NOAEL = 0.1% (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE